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Chapter 8: Application of Field-cycling ^{1}H NMR Relaxometry to the Study of Translational and Rotational Dynamics in Liquids and Polymers

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Abstract

© 2019 The Royal Society of Chemistry. With the availability of commercial field-cycling (FC) relaxometers together with progress in home-built instruments, NMR relaxometry has gained new momentum as a method of investigating the dynamics in complex liquids such as polymer melts or glass-forming systems. The method provides the dispersion of spin-lattice relaxation rate. Assuming frequencyerature superposition, master curves that extend up to 10 decades in amplitude and frequency are constructed from individual relaxation spectra measured at different temperatures. In the case of protons, due to the intra- and intermolecular origin of the dipolar interactions, relaxation dispersion reflects both rotational and translational dynamics. The latter displays a universal low-frequency dispersion law that allows the determination of the diffusion coefficient D in addition to the rotational time constant, i.e. FC-1H NMR becomes an alternative to field-gradient NMR. Sub-diffusive translation found in polymers is accessed by singling out the intermolecular relaxation via isotope dilution experiments. The mean square displacement was revealed to be a function of time, thus complementing neutron scattering experiments. Likewise, information on segmental reorientational dynamics is provided by the intramolecular relaxation. Thereby, thorough testing of current polymer theories becomes possible.

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References

[1] F. Noack Prog. NMR Spectrosc. 1986 18 171
[2] R. Kimmich E. Anoardo Prog. NMR Spectrosc. 2004 44 257
[3] D. Kruk A. Herrmann E. A. Rössler Prog. NMR Spectrosc. 2012 63 33
[4] R. Meier D. Kruk E. A. Rössler ChemPhysChem 2013 14 3071
[5] E. A. Rössler S. Stapf N. Fatkullin Curr. Opin. Colloid Interface Sci. 2013 18 173
[6] F. Fujara D. Kruk A. F. Privalov Prog. NMR Spectrosc. 2014 82 39
[7] N. Fatkullin S. Stapf M. Hofmann R. Meier E. A. Rössler J. Non-Cryst. Solids 2015 407 309
[8] R. Kimmich N. Fatkullin Progr. NMR Spectrosc. 2017 101 18
[9] R. B. Steele J.-P. Korb G. Ferrante S. Bubici Magn. Reson. Chem. 2016 54 502
[10] STELAR Company: www.stelar.it
[11] B. Kresse A. F. Privalov F. Fujara Solid State Nucl. Magn. Reson. 2011 40 134
[12] A. Herrmann B. Kresse J. Gmeiner A. Privalov D. Kruk F. Fujara E. A. Rössler Macromolecules 2012 45 1408
[13] B. Kresse A. F. Privalov A. Herrmann M. Hofmann E. A. Rössler F. Fujara Solid State Nucl. Magn. Reson. 2014 59 45

[14] M. Hofmann B. Kresse L. Heymann A. F. Privalov L. Willner N. Fatkullin N. Aksel F. Fujara E. A. Rössler Macromolecules 2016 49 8622

[15] V. Zampetoulas D. J. Lurie L. M. Broche J. Magn. Reson. 2017 282 38

[16] B. Kresse M. Becher A. F. Privalov M. Hofmann E. A. Rössler M. Vogel F. Fujara J. Magn. Reson. 2017 277 79

[17] D. M. Sousa P. A. L. Fernandes G. D. Marques A. C. Ribeiro P. J. Sebastiao Solid State Magn. Reson. 2010 25 160

[18] S. Korchak K. Ivanov A. Yurkovskaya H.-M. Vieth J. Chem. Phys. 2012 133 094502

[19] S. Kruber G. D. Farrher E. Anoardo J. Magn. Reson. 2015 259 216

[20] O. Neudert C. Mattea S. Stapf J. Magn. Reson. 2016 271 7

[21] C. Y. Chou M. Abdesselem C. Bouzigues M. Chu A. Guiga T.H. Huang F. Ferrage T. Gacoin A. Alexandrou D. Sakellariou Sci. Rep. 2017 7 44770

[22] L. Trahms M. Burghoff J. Magn. Reson. Imaging 2010 28 1244

[23] S. Stapf R. Kimmich R. O. Seiter Phys. Rev. Lett. 1995 75 2855

[24] D. Kruk R. Meier A. Rachocki A. Korpała R. K. Singh E. A. Rössler J. Chem. Phys. 2014 140 244509

[25] A. O. Seyedlar S. Stapf C. Mattea Phys. Chem. Chem. Phys. 2015 17 1633

[26] M. Kehr N. Fatkullin R. Kimmich J. Chem. Phys. 2007 127 084911

[27] M. Flämig M. Becher M. Hofmann T. Körber B. Kresse A. F. Privalov L. Willner D. Kruk F. Fujara E. A. Rössler J. Phys. Chem. B 2016 120 7754

[28] A. Abragam, The Principles of Nuclear Magnetism, Clarendon Press, Oxford, 1961

[29] W. S. Price, NMR Studies of Translational Motion, Cambridge University Press, Cambridge 2009

[30] N. Fatkullin A. Gubaidullin C. Mattea S. Stapf J. Chem. Phys. 2013 137 224907

[31] A. Lozovoi C. Mattea A. Herrmann E. A. Rössler S. Stapf N. Fatkullin J. Chem. Phys. 2016 144 241101

[32] F. Furtado J. Damron M.-L. Trutschel C. Franz K. Schröter R. C. Ball K. Saalwächter D. Panja Macromolecules 2014 47 256

[33] A. Lozovoi C. Mattea M. Hofmann K. Saalwächter N. Fatkullin S. Stapf J. Chem. Phys. 2017 146 224901

[34] A. Lozovoi L. Petrova C. Mattea E. A. Rössler S. Stapf N. Fatkullin J. Chem. Phys. 2017 147 074904

[35] R. Kimmich N. Fatkullin Adv. Polym. Sci. 2004 170 1

[36] M. Kehr N. Fatkullin R. Kimmich J. Chem. Phys. 2007 126 094903

[37] D. Wolf, Spinerature and Nuclear-Spin Relaxation in Matter: basic principles and applications, Clarendon Press, Oxford 1979

[38] N. Bloembergen E. M. Purcell R. V. Pound Phys. Rev. 1948 73 679

[39] C. J. F. Böttcher and P. Bordewijk, Theory of Electric Polarization, Elsevier Scientific, Amsterdam 1978, vol. II

[40] P. Lunkenheimer U. Schneider R. Brand A. Loidl Contemp. Phys. 2000 41 15

[41] N. Petzold B. Schmidtke R. Kahlau D. Bock B. Micko R. Meier D. Kruk E. A. Rössler J. Chem. Phys. 2013 138 154501

[42] H. C. Torrey Phys. Rev. 1953 92 962

[43] L. P. Hwang J. H. Freed J. Chem. Phys. 1975 63 4017

[44] Y. Ayant E. Beloritzky J. Alizon J. Gallice J. Phys. 1975 36 991

[45] C. A. Sholl J. Phys. C: Solid State Phys. 1981 14 447

[46] J. Kowalewski and L. Mäler, Nuclear Spin Relaxation in Liquids: Theory, Experiments, and Applications, Taylor & Francis, New York 2006

[47] D. Kruk R. Meier E. A. Rössler J. Phys. Chem. B 2011 115 951

[48] Y. Ayant E. Belorizky P. Fries J. Rosset J. Phys. 1977 38 325

[49] P. Fries E. Belorizky J. Phys. 1978 39 1263

[50] J. P. Albrand M. C. Taieb P. H. Fries E. Beloritzky J. Chem. Phys. 1983 78 5809

[51] R. Meier D. Kruk A. Bourdick E. Schneider E. A. Rössler Appl. Magn. Reson. 2013 44 153

[52] R. Meier D. Kruk J. Gmeiner E. A. Rössler J. Chem. Phys. 2012 136 034508

[53] S. Kariyo C. Gainaru H. Schick A. Brodin V. N. Novikov E. A. Rössler Phys. Rev. Lett. 2006 97 207803

[54] A. Herrmann C. Gainaru H. Schick A. Brodin V. N. Novikov E. A. Rössler Phys. Rev. Lett. 2008 100 109901

[55] S. Kariyo A. Brodin C. Gainaru A. Herrmann H. Schick V. N. Novikov E. A. Rössler Macromolecules 2008 41 5313

[56] C. Gainaru O. Lips A. Troshagina R. Kahlau A. Brodin F. Fujara E. A. Rössler J. Chem. Phys. 2008 128 174505

[57] J. D. Ferry, Viscoelasticity Properties of Polymers, John Wiley & Sons Ltd., New York, 1980

[58] K. Binder and W. Kob, Glassy Materials and Disordered Solids, World Scientific, Singapore, 2005
[59] S. Kariyo S. Stapf Macromol. Chem. Phys. 2005 206 1300
[60] R. Kimmich N. Fatkullin R.-O. Seitter K. Gille J. Chem. Phys. 1998 108 2173
[61] D. Kruk R. Meier E. A. Roessler Phys. Rev. E 2012 85 020201
[62] H. E. Heinze H. Pfeifer Z. Phys. 1966 192 23
[63] J. F. Harmon B. H. Muller Phys. Rev. 1969 182 400
[64] E. Beloritzki P. H. Fries Chem. Phys. Lett. 1988 145 33
[65] A. Kuhn, P. Sreeraj, R. Pöttgen H.-D. Wiemhöfer, M. Wilkening and P. Heitjans, in Diffusion in Condensed Matter, Methods, Materials, Models, ed, P. Heitjans, and, J. Kärger, Springer, Berlin, 2005
[66] U. Stark E. Cebe K. Meise-Gresch W. Müller-Warmuth J. Mol. Liquids 1992 52 67
[67] R. Meier A. Herrmann M. Hofmann B. Schmidtke B. Kresse A. F. Privalov D. Kruk F. Fujara E. A. Rössler Macromolecules 2013 46 5538
[68] M. Hofmann C. Gainaru B. Cetinkaya R. Vaiullin N. Fatkullin E. A. Rössler Macromolecules 2015 48 7521
[69] A. O. Seyedlar S. Stapf C. Mattea Phys. Chem. Chem. Phys. 2017 121 5363
[70] M. Odelius A. Laaksonen M. H. Levitt J. Kowalewski J. Magn. Reson. 1993 A 105 289
[71] P. Henritzi A. Bormuth M. Vogel Solid State Nucl. Magn. Reson. 2013 54 32
[72] I. Chang H. Sillescu J. Phys. Chem. B 1997 101 8794
[73] R. Meier E. Schneider E. A. Rössler J. Chem. Phys. 2015 142 034503
[74] A. Herrmann B. Kresse M. Wohlfahrt I. Bauer A. F. Privalov D. Kruk N. Fatkullin F. Fujara E. A. Rössler Macromolecules 2012 45 6516
[75] S. Kariyo S. Stapf Solid State Nucl. Magn. Reson. 2004 25 64
[76] S. Kariyo A. Brodin C. Gainaru A. Herrmann J. Hintermeyer H. Schick V. N. Novikov E. A. Rössler Macromolecules 2008 41 5322
[77] A. Herrmann V. N. Novikov E. A. Rössler Macromolecules 2009 42 2063
[78] A. Herrmann S. Kariyo A. Abou Elfadl R. Meyer V. N. Novikov E. A. Rössler Macromolecules 2009 42 5236
[79] A. Bormuth M. Hofmann P. Henritzi M. Vogel E. A. Rössler Macromolecules 2013 46 7805
[80] M. Hofmann B. Kresse A. F. Privalov L. Willner N. Fatkullin F. Fujara E. A. Rössler Macromolecules 2014 47 7917
[81] B. Kresse M. Hofmann A. F. Privalov N. Fatkullin F. Fujara E. A. Rössler Macromolecules 2015 48 4491
[82] M. Hofmann A. Herrmann A. Abou Elfadl D. Kruk M. Wohlfahrt E. A. Rössler Macromolecules 2012 45 2390
[83] M. Hofmann B. Kresse A. F. Privalov L. Heymann L. Willner N. Aksel N. Fatkullin F. Fujara E. A. Rössler Macromolecules 2016 49 7945
[84] P. G. deGennes J. Chem. Phys. 1971 55 572
[85] M. Doi and S. F. Edwards, The Theory of PolymerDynamics, Science Publication, Oxford, London, 1986
[86] D. Richter, in Dynamics of Soft Matter, ed, V. G. Sakai, Ch. Alba-Simionesco, and, S.-H. Chen, Springer, New York, 2012
[87] K. S. Schweizer J. Chem. Phys. 1989 91 5802
[88] K. S. Schweizer M. Fuchs G. Szamel M. Guenza H. Tang Macromol. Theory Simul. 1997 6 1037
[89] N. Fatkullin R. Kimmich H.-W. Weber Phys. Rev. E 1993 47 4600
[90] M. A. Kroutieva N. F. Fatkullin R. Kimmich Polym. Sci., Ser. A 2005 47 1716
[91] N. Fatkullin R. Kimmich J. Chem. Phys. 1994 101 822
[92] R. C. Ball P. T. Callaghan E. T. Samulski J. Chem. Phys. 1997 106 7352
[93] Z. Wang A. E. Likhtman R. G. Larson Macromolecules 2012 45 3557
[94] R. Meier R. Kahlau D. Kruk E. A. Rössler J. Phys. Chem. A 2010 114 7847
[95] F. Fujara B. Geil H. Sillescu G. Z. Fleischer Z. Phys. B: Condens. Matter 1992 88 195
[96] A. Döß ig; M. Paluch H. Sillescu G. Hinze J. Chem. Phys. 2002 117 6582
[97] S. Schildmann A. Reiser R. Gainaru C. Gainaru R. Böhmer J. Chem. Phys. 2011 135 174511
[98] F. Furtado J. Damron M.-L. Trutschel C. Frany K. Schröter R. C. Ball K. Saalwächter D. Panja Macromolecules 2014 47 256
[99] F. Vaca Chávez K. Saalwächter Macromolecules 2011 44 1560
[100] A. Herrmann E. A. Rössler ACS Macro Lett. 1 1339
[101] M. Roos M. Hofmann S. Link M. Ott E. Rössler J. Balbach K. Saalwächter A. Krushelnitsky J. Biomol. NMR 2015 63 403

[102] M. Hofmann A. Herrmann S. Ok C. Franz D. Kruk Saalwächter M. Steinhart E. A. Rössler Macromolecules 2011 44 4017